



Methods for Using Anaconda on Personally Identifiable Information (PII)—Restricted Computers

by Dale Shires, Michael Frauenhoffer, and John Vines

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Methods for Using Anaconda on Personally Identifiable Information (PII)-Restricted Computers

Dale Shires, Michael Frauenhoffer, and John Vines

DEVCOM Army Research Laboratory

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
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1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE			3. DATES COVERED (From - To)
January 2023	Memorandum Rep	oort		11 August–11 October 2022
4. TITLE AND SUBTITLE	l			5a. CONTRACT NUMBER
Methods for Using Anaconda on Personally Identifi (PII)–Restricted Computers		able Information		5b. GRANT NUMBER
				5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)				5d. PROJECT NUMBER
Dale Shires, Michael Frauenhof	fer, and John Vines			
				5e. TASK NUMBER
				5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAM	E(S) AND ADDRESS(ES)			8. PERFORMING ORGANIZATION REPORT NUMBER
DEVCOM Army Research Labo	oratory			
ATTN: FCDD-RLA-DB	•			ARL-MR-1070
Aberdeen Proving Ground, MD	21005			
9. SPONSORING/MONITORING AGENC	Y NAME(S) AND ADDRES	SS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)
12. DISTRIBUTION/AVAILABILITY STAT	EMENT			
Approved for public release: dis	tribution unlimited.			
13. SUPPLEMENTARY NOTES				
14. ABSTRACT				
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15. SUBJECT TERMS				
Network, Cyber, and Computational Sciences; Anaconda; Python; machine learning; PII; Singularity; containers				
16. SECURITY CLASSIFICATION OF:		17. LIMITATION OF	18. NUMBER OF	19a. NAME OF RESPONSIBLE PERSON
		ABSTRACT	PAGES	Dale Shires

Standard Form 298 (Rev. 8/98) Prescribed by ANSI Std. Z39.18

19b. TELEPHONE NUMBER (Include area code)

(410) 278-5006

UU

33

a. REPORT

Unclassified

b. ABSTRACT

Unclassified

c. THIS PAGE

Unclassified

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1. Introduction

Anaconda is a Python/R data science distribution and collection of over 7,500 open-source packages that include a package and environment manager (Anaconda 2022). Anaconda can be downloaded and installed in the user's directory space on a computer system and does not necessarily require system administrator or "root" privileges to install. Anaconda can take a fair amount of disk space, so another related option is Miniconda, which only includes the Python interpreter and the package manager and thus reduces overall space requirements. Either software is platform-agnostic; you can install it on numerous operating systems to include Windows, Mac OS, and Linux. Anaconda environments can be created by way of command-line arguments or through the use of a YAML (YAML Ain't Markup Language) configuration file (often seen with a .yml extension) used to define all of the packages to install in the environment. An example YAML file is shown in Fig. 1.

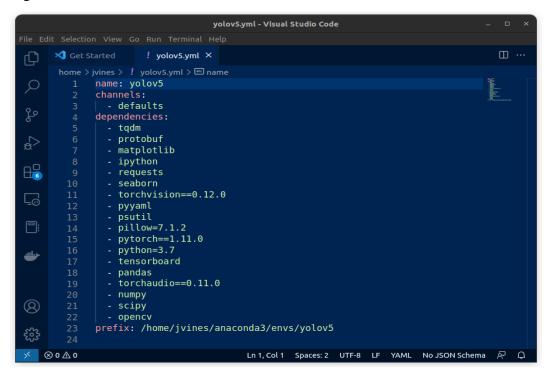


Fig. 1 An example YAML file

Once an Anaconda environment is created and activated, software developers can use the system to install specific versions of many machine learning (ML) packages, such as Pandas, NumPy, and PyTorch to name a few. Thereafter, these ML packages can easily be imported into Python software (code) to greatly simplify and speed the integration of approaches into customized software. Besides ML,

Anaconda supports a myriad of capabilities including neural networks, predictive analysis, and data visualization (anaconda.com 2022 [Oct 11]).

The software that Anaconda manages can be sourced from the Internet, hosted locally, or be from a file that exists on the local host. However, most often software is pulled from active Internet connections, and lacking this connection greatly complicates this process for obvious reasons. The authors recently encountered such a situation. One of the computer systems housed at the US Army Combat Capabilities Development Command (DEVCOM) Army Research Laboratory (ARL) was recently cleared to store and process personally identifiable information (PII), but as part of the process, Internet access was greatly curtailed. However, there are approaches to dealing with this problem, and these mitigation efforts are the focus of this report.

We discuss two ways to use Anaconda on systems with limited Internet connectivity. The first uses a concept of containers. Containers are useful for packaging all required software within itself to allow for installation and execution on varying system architectures. If the container software is supported on the development and target systems, the container can execute even if the development system differs from the target and deployed system.

The second method uses a concept of packing all the required software housed in an Anaconda environment into a library and then porting that library to a system with limited connectivity. This method only works when the development and target systems are based on similar architectures and operating systems.

For each of these approaches, we will assume that the Anaconda system has been installed in the user's directory. The methods to install "conda" (short for Anaconda) vary based on the underlying operating system and are covered in more detail on the Anaconda website (Anaconda 2022 [Oct 3]). Commands and prompts are usually listed in the Consolas font with the "\$" character as shell prompt.

2. Anaconda and Containers

There are numerous container runtimes (or engines) available today, to include Singularity and Podman among others. Determining which container system to use depends on a number of factors including functionality and ease-of-use for large-scale software deployment. We were looking mainly for a methodology to package and distribute Anaconda, so our criteria really came down to what was "easiest" and currently supported at the DOD Supercomputing Resource Center (DSRC). For these simple reasons, we chose to use Singularity. Like many container systems, Singularity requires a user to have root, or superuser, privileges to be most effective

during the build. To get around this problem, we utilized the Persistent Services Framework (PSF) running at the ARL DSRC (2021).

PSF is currently running on the system "Centennial" at the ARL DSRC. Once a user applies for access to PSF through the standard user-support system and is approved, an account is created on PSF, and the user can enjoy the ability to act as root while in the PSF environment. There are numerous configurations to address to get the overall system to function properly and there are many steps. We enumerate these in the following. In all cases we used Firefox web browser v. 102.3.0.

2.1 Initial Required Configurations

- 1) Acquire krb5 tickets. Use the High Performance Computing (HPC) Kerberos application to acquire login credentials and tickets.
- 2) Use putty to log into centennial15, which is the node where the PSF system is running. Also, putty must be configured properly for this approach to work. The first step is to configure the source and destination ports in the Secure Shell (SSH) Tunnels configuration. In the PuTTY configuration area, we chose to enter the value 5678 in the source port, and the destination we chose was localhost:7890. Once you enter those values in the appropriate fields, click the "Add" button. The window should appear as shown in Fig. 2. Proceed to log into the system on login node centennial15.

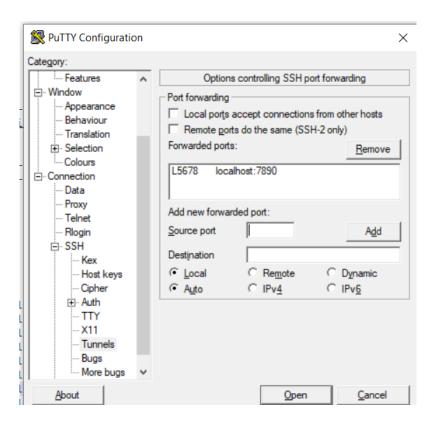


Fig. 2 PuTTY configuration for source and destination tunnel ports

3) Start a web browser. We chose to use the Firefox web browser for this test case. Update the connection settings by selecting the hamburger menu (or icon), select "Settings," then select "Network Settings." To match the settings we used in PuTTY, select the "Manual proxy configuration" option, and for SOCKS Host enter "localhost" with port number 5678. The radio button SOCKS v5 should be selected, and the option "Proxy DNS when using SOCKS v5" should also be enabled. The window should appear as shown in Fig. 3.

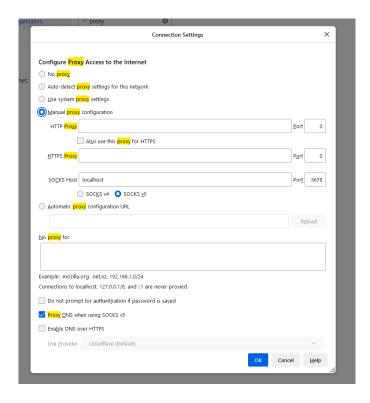


Fig. 3 Connection settings dialog box in Firefox

4) Log into the oVirt virtual machine (VM) manager at https://r6i4n0.ib0.arlu.arl.hpc.mil:8443/. You will need to supply your username and password created at the time of your PSF account creation. The oVirt interface will let you create, suspend, connect, and more to VMs in the PSF system. The login screen is shown in Fig. 4.

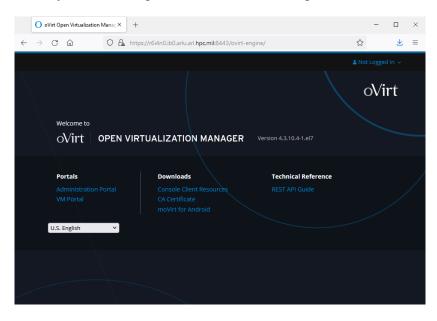


Fig. 4 oVirt login screen

5) Create a VM with standard default options. Here we created a VM called "test." When you click on the VM, the web page will display the summary state of the VM as shown in Fig. 5.

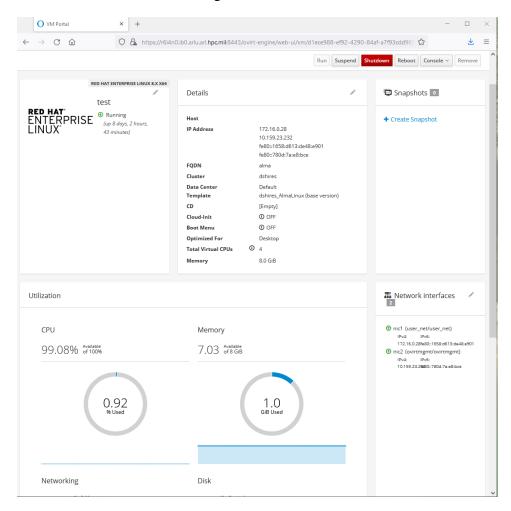


Fig. 5 Summary page for the VM "test"

6) Connect to the VM through a web browser. It is possible for the user to enter a terminal window via the console from the oVirt status page, but there is a Cockpit (https://cockpit-project.org/) version that has an enhanced look and feel that we chose to use for the remainder of this example. To use this, first determine the IP address for the VM from the Details section of the VM status page. From Fig. 6 we can see that the IP address is 10.159.23.232. To connect to the Cockpit interface, go to port 9090 by typing https://10.159.23.232:9090 in the address bar and hitting return. This will bring up the Cockpit interface as shown in Fig. 6.

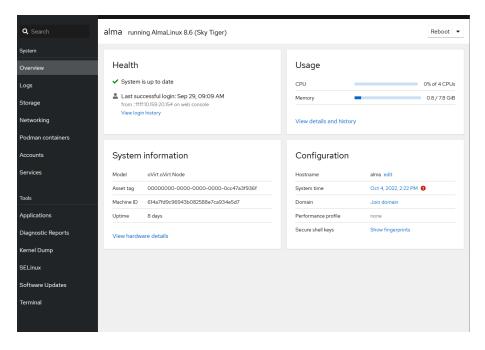


Fig. 6 Cockpit interface for the VM

7) Go into the terminal for this VM by selecting the "Terminal" tab in the Cockpit interface. Installing Anaconda and creating the Singularity container will be done through this terminal window.

2.2 Downloading and Installing Anaconda

Anaconda, or conda, can be installed for a variety of operating systems from the download page (Anaconda 2022 [Oct 3]). We are using systems at the ARL DSRC that use a mix of operating systems. Once conda is installed, the user proceeds by creating an environment, activating it, and then installing any required libraries into the environment. For example, suppose someone wants to create a new environment called "my_env" with the most recent version of Pandas (a data analysis library). From a system with Internet access, the following three commands would be entered:

- \$ conda create --name my_env
- 2) \$ conda activate my env
- 3) \$ conda install pandas

2.3 Iris Classification Test Case

For a test case, we wanted a relatively robust example that uses several Anaconda packages. The iris flower classification dataset provides this requirement, and there is a step-by-step tutorial online on how to build and test several models (machinelearningmastery.com 2020). We created an Anaconda environment called

"my_env." The libraries installed in the environment are listed using the "conda list" command and are shown in Appendix A – Output of "conda list." The Python source code is listed in Appendix B – iris.py, and the output of the software when executed natively on centennial is shown in Appendix C – Output of iris.py.

2.4 Creating, Testing, and Porting a Singularity Container

Using Anaconda inside of a container can be tricky. The first time an Anaconda environment is used, it must be initialized for the operating system in use, which in turn must be restarted for Anaconda to take effect. This rebooting step causes problems for Singularity containers. We discovered a good solution to this problem after quite a bit of searching online and by experimenting (csc-training.github.io 2022).

The first step is to export the working Anaconda environment to a YML file. From the operating system prompt, this is done by "conda env export > environment.yml". Next, create a Singularity definition file (in this case called iris.def), the contents of which appear as follows:

```
BootStrap: docker
From: continuumio/miniconda3
%help
        This is a container with conda environments and all materials required to run the
        Iris deep learning models.
%files
        environment.vml
        iris.csv
        iris.py
%environment
%post
        ENV NAME=$(head -1 environment.yml | cut -d ' ' -f2)
        echo ". /opt/conda/etc/profile.d/conda.sh" >> $SINGULARITY_ENVIRONMENT echo "conda activate $ENV_NAME" >> $SINGULARITY_ENVIRONMENT
         . /opt/conda/etc/profile.d/conda.sh
         conda env create -f environment.yml -p /opt/conda/envs/$ENV_NAME
        conda clean --all
        chmod 775 iris.csv
        chmod 775 iris.py
%runscript
        echo "Starting container runscript..."
        exec python /iris.py
```

Now this definition file, along with all the other files that are required to run the iris models, are placed in the same directory. (In this example we are using Singularity v. 3.8.7-1.el8.) It is not uncommon to run into issues regarding file and directory size limits when building containers, as they can become quite large. For instance, just using default path settings when building containers, we would often start to get errors that the build failed. Tracing back the reason revealed issues with size limits in our directory structure.

This can be corrected by using two Singularity environment variables: SINGULARITY_TMPDIR and SINGULARITY_CACHEDIR. Since the /home directory had plenty of available room, this directory can be specified for the build. Assuming a user named "joesmith" (for example), issue the following command to build the singularity container:

```
$ sudo SINGULARITY_TMPDIR=/home/joesmith/build/tmp
SINGULARITY_CACHEDIR=/home/joesmith/build/cache singularity build iris.sif iris.def
```

This will build the file iris.sif, where sif stands for Singularity Image Format. Note that building a container with several conda packages can take some time to complete.

We transferred this file to the system with PII storage that has limited Internet connectivity with an identical distribution of Singularity (v. 3.8.7-1.el8). Since there is a runscript defined in the iris.def build file, it is possible to change the file to executable (by issuing a chmod +x iris.sif command) and run it directly from the shell. We did this, and the output is listed in Appendix D on the destination computer. There is no randomization in the script, so the outputs of the two files do match, and the versions of the software modules loaded also match since they are self-contained within the container.

Note that is possible within the destination computer to now also enter a Singularity shell environment that will allow a user to write Python code and import those modules within the container, such as Pandas and NumPy. To do this, one needs to execute the command

\$ singularity shell iris.sif.

If other Anaconda modules are required, they will need to be installed on the source computer with a rebuilt container once again moved to the destination machine.

2.5 Possible Issues and Remedies with PSF

There is a lot of flexibility in the PSF environment; however, there are also many parameters and settings that might need to be adjusted due to things like the Defense Information Systems Agency Security Technical Implementation Guides, for instance. We list some of the possible items to look out for here:

• It is best to use the dnf command when installing software in PSF. Using dnf works with various security filters to allow the software to install properly. For example, to install Singularity the user would issue the command dnf install singularity. This command will update the whitelist of allowed commands.

- The file /etc/fstab in PSF might need to be modified to allow for execution privileges on various file systems. For example, if "noexec" is set on a file system, this will prevent code from executing directly from the media.
- If SELinux is active, it might interfere with some software installs or executions.

In those situations where there appears to be strange or hard-to-follow errors, it is best to be cautious and discuss the issue with a system administrator.

3. Anaconda and Conda-Pack

Conda-Pack is a utility that can be used when the development and target computers are of the same architecture type (Conda-Pack 2022). The most common use case is when the development computer has Python and Anaconda installed but the destination computer does not. This method requires a lot less work than the Singularity version and should be used whenever possible to simplify things.

The user must be connected to a terminal on the development computer where Anaconda is installed. This terminal could be the same as that described in Section 2 or simply a Linux terminal on the development computer. Downloading and installing Anaconda proceeds as described in Section 2.2. Conda-Pack should be installed in the root conda environment; that is, prior to issuing any conda activate commands. If an environment is currently active, conda deactivate should be done before Conda-Pack is installed.

Following the previous example, assume we have an environment called "my_env" that has all of the required Anaconda software to execute the iris.py file. The user issues the command conda pack -n my_env from the base environment as follows:

This creates the my_env.tar.gz file that is then ported by the user to the destination/target computer. The environment is unpacked into a new directory by issuing the following commands:

```
$ mkdir -p my_env
$ tar -xzf my_env.tar.gz -C my_env
```

Since we are only packing the environment, any other files that are required by the software, for instance in this case the iris.csv and iris.py files, also need to be moved

to the target computer. To mimic the Anaconda environment, we entered the following command:

\$ source my_env/bin/activate

Then we ran the iris.py Python code with the output given in Appendix E when using Conda-Pack. Note that the code generates the same results as other versions listed. To deactivate the environment and remove it from your path, enter the following command:

\$ source my_env/bin/deactivate

4. Conclusion

The ability to build on prior work and bring in already-built software libraries and routines greatly simplifies the life of a data scientist. Processing datasets that store PII data can be difficult, however, since computer systems may be behind firewalls and other protections that limit the ability to actively download required libraries that data scientists use often. There are at least two ways to deal with this problem, as discussed in this report. We hope that this discussion fast-tracks the use of Anaconda and its data science and ML tools in difficult processing situations such as those encountered when working with PII data.

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Appendix A. Output of "conda list"

```
# Name
                       Version
                                                Build Channel
_libgcc mutex
                        0.1
                                                  main
                                                         defaults
                       5.1
_openmp mutex
                                                          defaults
                                                 1_gnu
tflow select
                       2.3.0
                                                  mkl
                                                         defaults
                       20211102.0
abseil-cpp
                                           hd4dd3e8 0
                                                        defaults
absl-py
                       0.15.0
3.8.1
                                          pyhd3eb1b0 0
                                                         defaults
aiohttp
                                        py310h7f8727e 1
                                                         defaults
                       1.2.0
aiosignal
                                         pyhd3eb1b0 0
                                                         defaults
                       1.6.3
                                          py_0
pyhd3eb1b0 0
astunparse
                                                         defaults
async-timeout
                        4.0.1
                                                         defaults
                                          pyhd3eb1b0 0
attrs
                       21.4.0
                                                         defaults
                                                         defaults
blas
                        1.0
                                                   mkl
blinker
                                        py310h06a4308 0
                                                          defaults
                        1.4
                       1.3.5
                                       py310ha9d4c09 0
bottleneck
                                                         defaults
brotli
                       1.0.9
                                            h5eee18b 7
                                                          defaults
                                            h5eee18b_7
                       1.0.9
brotli-bin
                                                         defaults
brotlipy
                                        py310h7f8727e 1002 defaults
                       1.0.8
                                          h7b6447c 0
bzip2
                                                        defaults
                     1.18.1
2022.07.19
4.2.2
                                            h7f8727e 0
                                                          defaults
c-ares
ca-certificates
                                            h06a4308 0
                                                         defaults
cachetools
                                          pyhd3eb1b0 0
                                                         defaults
certifi
                       2022.6.15
                                        py310h06a4308 0
                                                         defaults
                       1.15.1
                                       py310h74dc2b5_0
pyhd3eb1b0_0
cffi
                                                          defaults
charset-normalizer
                                                         defaults
clang-14
                       14.0.6
                                       default hc1a23ef 0 defaults
                       8.0.4
                                      py310h06a4308_0 defaults
click
                                      py310h9ce1e76 0
cryptography
                        37.0.1
                                                         defaults
                                       pyhd3eb1b0_0
pyh6d0b6a4_7
                        0.11.0
                                                         defaults
cvcler
dataclasses
                       0.8
                                                         defaults
                       1.13.18
dbus
                                           hb2f20db_0
                                                         defaults
expat
                        2.4.4
                                            h295c915 0
                                                         defaults
                                            h27cfd23 1
fftw
                        3.3.9
                                                         defaults
flatbuffers
                       2.0.0
                                           h2531618 0
                                                          defaults
                       2.13.1
fontconfig
                                            h6c09931 0
                                                          defaults
                                          pyhd3eb1b0 0
fonttools
                                                         defaults
freetype
                       2.11.0
                                           h70c0345 0
                                                         defaults
                       1.2.0
0.5.3
                                       py310h7f8727e_1
pyhd3eb1b0_0
frozenlist
                                                          defaults
gast
                                                         defaults
                       5.2.1
                                            h7b6447c 0
aiflib
                                                         defaults
glib 2.69.1 google-auth 2.6.0 google-auth-oauthlib 0.4.4 google-pasta 0.2.0
glib
                       2.69.1
                                            h4ff587b 1
                                                         defaults
                                          pyhd3eb1b0_0
pyhd3eb1b0_0
                                                          defaults
                                                         defaults
                                          pyhd3eb1b0 0
                                                         defaults
                        1.46.1
                                                          defaults
grpc-cpp
                                            h33aed49 0
grpcio
                        1.42.0
                                        py310hce63b2e 0
                                                         defaults
gst-plugins-base
                       1.14.0
                                           h8213a91 2
                                                         defaults
gstreamer
                        1.14.0
                                            h28cd5cc 2
                                                          defaults
h5py
                        3.7.0
                                        py310he06866b 0
                                                          defaults
                                            h3ffc7dd 1
                                                         defaults
hdf5
                        1.10.6
                        58.2
icu
                                            he6710b0 3
                                                         defaults
                       3.3
4.11.3
                                          pyhd3eb1b0_0
                                                          defaults
idna
                                       py310h06a4308 0
importlib-metadata
                                                         defaults
                    4.11.3 2021.4.0
                                        h06a4308 3561
intel-openmp
                                                         defaults
joblib
                       1.1.0
                                         pyhd3eb1b0 0
                                                         defaults
                       9e
2.8.0
                                       h7f8727e_0
py310h06a4308 0
jpeg
                                                         defaults
keras
                                                         defaults
                    1.1.2
                                         pyhd3eb1b0 0
                                                         defaults
keras-preprocessing
kiwisolver
                                        py310h295c915_0
                                                          defaults
krb5
                        1.19.2
                                            hac12032 0
                                                          defaults
                                            h3be6417 0
1cms2
                       2.12
                                                          defaults
ld impl linux-64
                       2.38
                                            h1181459 1
                                                          defaults
                       3.0
1.0.9
1.0.9
lerc
                                            h295c915 0
                                                          defaults
libbrotlicommon
                                            h5eee18b 7
                                                         defaults
libbrotlidec
                                            h5eee18b 7
                                                         defaults
                    1.0.9
10.0.1
14.0.6
7.84.0
libbrotlienc
                                                         defaults
                                            h5eee18b 7
                       10.0.1
libclang
                                        default hb85057a 2 defaults
                                        default hc1a23ef 0
libclang-cpp14
                                                            defaults
libcurl
                       7.84.0
                                           h91b91d3 0
                                                        defaults
libdeflate
                        1.8
                                            h7f8727e_5
                                                          defaults
libedit.
                        3.1.20210910
                                            h7f8727e 0
                                                         defaults
                                            h7f8727e 1
libev
                        4.33
                                                       defaults
```

libevent	2.1.12	h8f2d780_0	defaults
libffi	3.3	he6710b0 2	defaults
libgcc-ng	11.2.0	h1234567 ⁻ 1	defaults
libgfortran-ng	11.2.0	h00389a5 1	defaults
libgfortran5	11.2.0	h1234567 1	defaults
		_	
libgomp	11.2.0	h1234567_1	defaults
libllvm10	10.0.1	hbcb73fb_5	defaults
libllvm14	14.0.6	hef93074 0	defaults
libnghttp2	1.46.0	hce63b2e 0	defaults
libpng	1.6.37	hbc83047 0	defaults
libpq	12.9	h16c4e8d 3	defaults
		_	
libprotobuf	3.20.1	h4ff587b_0	defaults
libssh2	1.10.0	h8f2d780_0	defaults
libstdcxx-ng	11.2.0	h1234567_1	defaults
libtiff	4.4.0	hecacb30 0	defaults
libuuid	1.0.3	h7f8727e 2	defaults
libwebp	1.2.2	h55f646e 0	defaults
±		-	defaults
libwebp-base	1.2.2	h7f8727e_0	
libxcb	1.15	h7f8727e_0	defaults
libxkbcommon	1.0.1	hfa300c1_0	defaults
libxml2	2.9.14	h74e7548 0	defaults
libxslt	1.1.35	h4e12654 0	defaults
lz4-c	1.9.3	h295c915 1	defaults
markdown	3.3.4	py310h06a4308 0	defaults
matplotlib	3.5.2	py310h06a4308_0	defaults
matplotlib-base	3.5.2	py310hf590b9c_0	defaults
mkl	2021.4.0	h06a4308 640	defaults
mkl-service	2.4.0	py310h7f8727e 0	defaults
mkl fft	1.3.1	py310hd6ae3a3 0	defaults
_	1.2.2	py310h00e6091 0	defaults
mkl_random		-	
multidict	5.2.0	py310h5eee18b_3	defaults
munkres	1.1.4	ру_0	defaults
ncurses	6.3	h5eee18b 3	defaults
nltk	3.7	pyhd3eb1b0 0	defaults
nspr	4.33	h295c915 0	defaults
nss	3.74	h0370c37 0	defaults
		-	
numexpr	2.8.3	py310hcea2de6_0	defaults
numpy	1.22.3	py310hfa59a62_0	defaults
numpy-base	1.22.3	py310h9585f30_0	defaults
oauthlib	3.2.0	pyhd3eb1b0 1	defaults
openssl	1.1.1q	h7f8727e 0	defaults
opt_einsum	3.3.0	pyhd3eb1b0 1	defaults
	21.3		defaults
packaging		pyhd3eb1b0_0	
pandas	1.4.3	py310h6a678d5_0	defaults
pcre	8.45	h295c915_0	defaults
pillow	9.2.0	py310hace64e9 1	defaults
pip	22.1.2	py310h06a4308 0	defaults
ply	3.11	py310h06a4308 0	defaults
protobuf	3.20.1	py310h295c915 0	defaults
=			
pyasn1	0.4.8	pyhd3eb1b0_0	defaults
pyasn1-modules	0.2.8	py_0	defaults
pycparser	2.21	pyhd3eb1b0_0	defaults
pyjwt	2.4.0	py310h06a4308 0	defaults
pyopenssl	22.0.0	pyhd3eb1b0 0	defaults
pyparsing	3.0.9	py310h06a4308 0	defaults
	5.15.7	py310h6a678d5 1	defaults
pyqt			
pyqt5-sip	12.11.0	pypi_0	pypi
pysocks	1.7.1	py310h06a4308_0	defaults
python	3.10.4	h12debd9 0	defaults
python-dateutil	2.8.2	pyhd3eb1b0 0	defaults
python-flatbuffers	2.0	pyhd3eb1b0 0	defaults
pytz	2022.1	py310h06a4308 0	defaults
pyyaml	6.0	pypi_0	pypi
qt-main	5.15.2	h327a75a_7	defaults
qt-webengine	5.15.9	hd2b0992_4	defaults
qtwebkit	5.212	h4eab89a 4	defaults
re2	2022.04.01	h295c915 0	defaults
readline	8.1.2	h7f8727e 1	defaults
		-	
regex	2022.7.9	py310h5eee18b_0	defaults
requests	2.28.1	py310h06a4308_0	defaults
requests-oauthlib	1.3.0	bA ⁰	defaults

rsa scikit-learn scipy setuptools sip six snappy sqlite tensorboard tensorboard-data-server tensorboard-plugin-wit tensorflow tensorflow-base tensorflow-estimator termcolor threadpoolctl tk toml tornado tqdm typing-extensions typing_extensions tzdata urllib3 werkzeug wheel wrapt xz yaml yarl zipp	4.7.2 1.1.1 1.7.3 63.4.1 6.6.2 1.16.0 1.1.9 3.39.2 2.8.0 0.6.0 1.8.1 2.8.2 2.8.2 2.8.0 1.1.0 2.2.0 8.6.12 0.10.2 6.2 4.64.0 4.3.0 4.3.0 2022a 1.26.11 2.0.3 0.37.1 1.14.1 5.2.5 0.2.5 1.8.1 3.8.0	pyhd3eb1b0_1 py310h6a678d5_0 py310h1794996_2 py310h06a4308_0 py310h6a678d5_0 pyhd3eb1b0_1 h295c915_0 h5082296_0 py310h06a4308_0 py310h06a4308_0 py310h06a4308_0 mk1_py310hd2b8f8c mk1_py310h684308_1 py310h64308_1 py40d69192_0 h1ccaba5_0 py310h06a4308_0 py1006a4308_0	
=		_	
=			
zlib	1.2.12	h7f8727e_2	defaults
zstd	1.5.2	ha4553b6_0	defaults

Appendix B. Python Script: iris.py

```
# This is a test of using conda and ML libraries in general in PSF.
# See https://machinelearningmastery.com/machine-learning-in-python-step-by-step/
import sys
print('Python: {}'.format(sys.version))
import scipy
print('scipy: {}'.format(scipy. version ))
import numpy
print('numpy: {}'.format(numpy.__version__))
import matplotlib
print('matplotlib: {}'.format(matplotlib. version ))
import pandas
print('pandas: {}'.format(pandas. version ))
import sklearn
print('sklearn: {}'.format(sklearn. version ))
# Load required libraries
from pandas import read csv
from pandas.plotting import scatter matrix
from matplotlib import pyplot
from sklearn.model selection import train test split
{\tt from \ sklearn.model\_selection \ import \ cross\_val\_score}
from sklearn.model_selection import StratifiedKFold
from sklearn.metrics import classification report
from sklearn.metrics import confusion_matrix
from sklearn.metrics import accuracy score
from sklearn.linear model import LogisticRegression
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.discriminant analysis import LinearDiscriminantAnalysis
from sklearn.naive bayes import GaussianNB
from sklearn.svm import SVC
# Load dataset
names = ['sepal-length', 'sepal-width', 'petal-length', 'petal-width', 'class']
dataset = read csv('/iris.csv', names=names)
# Summarize the dataset
# There should be 150 instances and 5 attributes
print(dataset.shape)
print (dataset.head(20))
print(dataset.describe())
# Class distribution
print(dataset.groupby('class').size())
# Split out validation dataset
array = dataset.values
X = array[:, 0:4]
y = array[:,4]
X train, X validation, Y train, Y validation = train test split(X, y,
test size=0.20, random state=1)
models = []
models.append(('LR', LogisticRegression(solver='liblinear', multi class='ovr')))
models.append(('LDA', LinearDiscriminantAnalysis()))
models.append(('KNN', KNeighborsClassifier()))
models.append(('CART', DecisionTreeClassifier()))
models.append(('NB', GaussianNB()))
models.append(('SVM', SVC(gamma='auto')))
# Evaluate each model in turn
results = []
names = []
for name, model in models:
        kfold = StratifiedKFold(n splits=10, random state=1, shuffle=True)
        cv_results = cross_val_score(model, X_train, Y train, cv=kfold,
scoring='accuracy')
        results.append(cv results)
        names.append(name)
```

```
print('%s: %f (%f)' % (name, cv_results.mean(), cv_results.std()))

# Make predictions on validation dataset
model = SVC(gamma='auto')
model.fit(X_train, Y_train)
predictions = model.predict(X_validation)

# Evaluate predictions
print(accuracy_score(Y_validation, predictions))
print(confusion_matrix(Y_validation, predictions))
print(classification_report(Y_validation, predictions))
```

Appendix C. Output of iris.py on Source Computer

```
Python: 3.10.4 (main, Mar 31 2022, 08:41:55) [GCC 7.5.0]
scipy: 1.7.3
numpy: 1.22.3
matplotlib: 3.5.2
pandas: 1.4.3
sklearn: 1.1.1
(150, 5)
    sepal-length sepal-width petal-length petal-width
                   3.5
                                             0.2 Iris-setosa
0.2 Iris-setosa
0
                                  1.4
             5.1
1
             4.9
                          3.0
                                        1.4
                                                    0.2 Iris-setosa
2
             4.7
                          3.2
                                       1.3
                                       1.5
1.4
1.7
                                                    0.2 Iris-setosa
0.2 Iris-setosa
0.4 Iris-setosa
3
             4.6
                         3.1
             5.0
                          3.6
4
                          3.9
5
             5.4
                                       1.4
1.5
1.4
             4.6
                         3.4
                                                     0.3 Iris-setosa
                                                     0.2 Iris-setosa
7
             5.0
                         3.4
8
             4.4
                          2.9
                                                     0.2
                                                          Iris-setosa
                                       1.5
                                                     0.1 Iris-setosa
9
            4.9
                         3.1
10
            5.4
                         3.7
                                       1.5
                                                     0.2 Iris-setosa
                         3.4
3.0
                                       1.6
1.4
                                                     0.2 Iris-setosa
0.1 Iris-setosa
11
             4.8
12
            4.8
13
            4.3
                         3.0
                                       1.1
                                                     0.1 Iris-setosa
                                                     0.2 Iris-setosa
0.4 Iris-setosa
                                       1.2
1.5
14
             5.8
                         4.0
15
             5.7
                         4.4
                                       1.3
                                                     0.4 Iris-setosa
16
             5.4
                         3.9
17
             5.1
                         3.5
                                       1.4
                                                     0.3 Iris-setosa
                                                     0.3 Iris-setosa
0.3 Iris-setosa
18
             5.7
                          3.8
                                        1.7
                                       1.5
19
             5.1
                          3.8
       sepal-length sepal-width petal-length petal-width
       150.000000 150.000000 150.000000 150.000000
count.
mean
          5.843333
                        3.054000
                                    3.758667
                                                   1.198667
           0.828066
                        0.433594
                                      1.764420
                                                   0.763161
std
          4.300000
                                     1.000000
min
                        2.000000
                                                   0.100000
           5.100000
                        2.800000
                                      1.600000
25%
                                                   0.300000
50%
          5.800000
                        3.000000
                                      4.350000
                                                   1.300000
75%
          6.400000
                       3.300000
                                      5.100000
                                                  1.800000
          7.900000
                        4.400000
                                      6.900000
                                                   2.500000
max
class
Iris-setosa
                   50
Iris-versicolor
                   50
Iris-virginica
dtype: int64
LR: 0.941667 (0.065085)
LDA: 0.975000 (0.038188)
KNN: 0.958333 (0.041667)
CART: 0.950000 (0.040825)
NB: 0.950000 (0.055277)
SVM: 0.983333 (0.033333)
0.9666666666666667
[[11 0 0]
 [ 0 12 1]
 [ 0 0 6]]
                            recall f1-score support
                 precision
    Tris-setosa
                      1.00
                                1.00
                                          1.00
                                                       11
Iris-versicolor
                      1.00
                                0.92
                                          0.96
                                                       13
                      0.86
                                1.00
                                          0.92
Iris-virginica
                                                       6
                                          0.97
                                                       30
       accuracy
      macro avg
                      0.95
                                0.97
                                          0.96
                                                      30
   weighted avg
                      0.97
                                0.97
                                          0.97
                                                      30
```

Appendix D. Output of iris.py on Destination Computer

```
Starting container runscript...
Python: 3.10.4 (main, Mar 31 2022, 08:41:55) [GCC 7.5.0]
scipy: 1.7.3
numpy: 1.22.3
matplotlib: 3.5.2
pandas: 1.4.3
sklearn: 1.1.1
(150, 5)
    sepal-length sepal-width petal-length petal-width
                                                                 class
                                              0.2 Iris-setosa
0
             5.1
                    3.5
                                 1.4
                                                     0.2 Iris-setosa
1
             4.9
                          3.0
                                        1.4
2
             4.7
                          3.2
                                        1.3
                                                     0.2 Iris-setosa
                                                     0.2 Iris-setosa
0.2 Iris-setosa
3
             4.6
                          3.1
                                        1.5
                          3.6
                                       1.4
4
             5.0
5
             5.4
                          3.9
                                       1.7
                                                     0.4 Iris-setosa
                                                     0.3 Iris-setosa
6
             4.6
                          3.4
                                        1.4
7
             5.0
                          3.4
                                        1.5
                                                     0.2
                                                          Iris-setosa
                                                     0.2 Iris-setosa
8
             4.4
                         2.9
                                        1.4
9
             4.9
                         3.1
                                        1.5
                                                     0.1 Iris-setosa
                                                     0.2 Iris-setosa
0.2 Iris-setosa
10
             5.4
                          3.7
                                        1.5
                                       1.6
11
             4.8
                          3.4
12
             4.8
                         3.0
                                       1.4
                                                     0.1 Iris-setosa
                                                     0.1 Iris-setosa
0.2 Iris-setosa
                                        1.1
1.2
13
             4.3
                          3.0
14
             5.8
                          4.0
                                                     0.4 Iris-setosa
15
             5.7
                         4.4
                                       1.5
16
             5.4
                         3.9
                                       1.3
                                                     0.4 Iris-setosa
                                                     0.3 Iris-setosa
0.3 Iris-setosa
17
             5.1
                          3.5
                                        1.4
             5.7
                                        1.7
18
                          3.8
19
             5.1
                          3.8
                                       1.5
                                                      0.3 Iris-setosa
       sepal-length sepal-width petal-length petal-width
        150.000000
                     150.000000
                                   150.000000
                                                 150.000000
count
           5.843333
                       3.054000
                                     3.758667
                                                   1.198667
mean
std
           0.828066
                        0.433594
                                      1.764420
                                                    0.763161
           4.300000
                        2.000000
                                      1.000000
min
                                                   0.100000
2.5%
           5.100000
                        2.800000
                                      1.600000
                                                   0.300000
50%
           5.800000
                        3.000000
                                      4.350000
                                                   1.300000
                                      5.100000
           6.400000
                        3.300000
75%
                                                   1.800000
max
           7.900000
                        4.400000
                                      6.900000
                                                   2.500000
class
Iris-setosa
                   50
Iris-versicolor
                   50
Iris-virginica
                   50
dtype: int64
LR: 0.941667 (0.065085)
LDA: 0.975000 (0.038188)
KNN: 0.958333 (0.041667)
CART: 0.950000 (0.055277)
NB: 0.950000 (0.055277)
SVM: 0.983333 (0.033333)
0.966666666666667
[[11 0 0]
[ 0 12 1]
 [ 0 0 6]]
                 precision
                            recall f1-score
                                                 support
                                1.00
                                          1.00
    Iris-setosa
                      1.00
                                                       11
                      1.00
                                0.92
                                          0.96
Iris-versicolor
                                                       13
                      0.86
                                1.00
                                          0.92
 Iris-virginica
                                                        6
                                          0.97
                                                       30
       accuracy
      macro avg
                      0.95
                                0.97
                                          0.96
                                                       30
                      0.97
   weighted avg
                                0.97
                                          0.97
                                                       30
```

Appendix E. Output of iris.py when Using Conda-Pack

```
Python: 3.8.13 (default, Mar 28 2022, 11:38:47)
[GCC 7.5.0]
scipy: 1.7.3
numpy: 1.21.5
matplotlib: 3.5.2
pandas: 1.4.4
sklearn: 1.1.1
(150, 5)
    sepal-length sepal-width petal-length petal-width
                                                                class
                                              0.2 Iris-setosa
0
             5.1
                    3.5
                                 1.4
                                                     0.2 Iris-setosa
1
             4.9
                          3.0
                                        1.4
2
             4.7
                          3.2
                                        1.3
                                                     0.2 Iris-setosa
3
             4.6
                          3.1
                                        1.5
                                                     0.2
                                                          Iris-setosa
                                                     0.2 Iris-setosa
                          3.6
                                       1.4
4
             5.0
5
             5.4
                          3.9
                                       1.7
                                                     0.4 Iris-setosa
6
             4.6
                          3.4
                                        1.4
                                                     0.3 Iris-setosa
7
             5.0
                          3.4
                                        1.5
                                                     0.2
                                                          Iris-setosa
                                                     0.2 Iris-setosa
8
             4.4
                          2.9
                                        1.4
9
             4.9
                          3.1
                                        1.5
                                                     0.1 Iris-setosa
                                                     0.2 Iris-setosa
0.2 Iris-setosa
10
             5.4
                          3.7
                                        1.5
                                       1.6
11
             4.8
                          3.4
12
             4.8
                          3.0
                                       1.4
                                                     0.1 Iris-setosa
                                                     0.1 Iris-setosa
0.2 Iris-setosa
                          3.0
13
             4.3
                                        1.1
14
             5.8
                          4.0
                                        1.2
                                                     0.4 Iris-setosa
15
             5.7
                         4.4
                                       1.5
16
             5.4
                         3.9
                                       1.3
                                                     0.4 Iris-setosa
                                                     0.3 Iris-setosa
0.3 Iris-setosa
17
             5.1
                          3.5
                                        1.4
             5.7
                          3.8
                                        1.7
18
19
             5.1
                          3.8
                                       1.5
                                                     0.3 Iris-setosa
       sepal-length sepal-width petal-length petal-width
        150.000000
                     150.000000
                                   150.000000
                                                 150.000000
count
           5.843333
                       3.054000
                                     3.758667
                                                   1.198667
mean
           0.828066
std
                        0.433594
                                      1.764420
                                                   0.763161
           4.300000
                        2.000000
                                      1.000000
                                                   0.100000
min
25%
           5.100000
                        2.800000
                                      1.600000
                                                   0.300000
50%
           5.800000
                        3.000000
                                      4.350000
                                                   1.300000
                        3.300000
                                      5.100000
           6.400000
                                                   1.800000
75%
max
           7.900000
                        4.400000
                                      6.900000
                                                   2.500000
class
Iris-setosa
                   50
Iris-versicolor
                   50
Iris-virginica
                   50
dtype: int64
LR: 0.941667 (0.065085)
LDA: 0.975000 (0.038188)
KNN: 0.958333 (0.041667)
CART: 0.941667 (0.038188)
NB: 0.950000 (0.055277)
SVM: 0.983333 (0.033333)
0.9666666666666667
[[11 0 0]
[ 0 12 1]
 [ 0 0 6]]
                 precision
                            recall f1-score
                                                 support
                                1.00
                                          1.00
    Iris-setosa
                      1.00
                                                       11
                      1.00
                                0.92
                                          0.96
Iris-versicolor
                                                       13
                      0.86
                                1.00
                                          0.92
 Iris-virginica
                                                       6
                                          0.97
                                                      30
       accuracy
      macro avg
                      0.95
                                0.97
                                          0.96
                                                       30
                      0.97
                                0.97
                                          0.97
   weighted avg
                                                      30
```

List of Symbols, Abbreviations, and Acronyms

ARL Army Research Laboratory

conda Anaconda

DEVCOM US Army Combat Capabilities Development Command

DNS Domain Name System

DOD Department of Defense

DSRC DOD Supercomputing Resource Center

HPC High Performance Computing

IP Internet Protocol

ML machine learning

OS operating system

PII personally identifiable information

PSF Persistent Services Framework

sif Singularity Image Format

SSH Secure Shell

VM virtual machine

YAML YAML Ain't Markup Language

YML YAML file

1 DEFENSE TECHNICAL

(PDF) INFORMATION CTR DTIC OCA

1 DEVCOM ARL

(PDF) FCDD RLB CI TECH LIB

3 DEVCOM ARL

(PDF) FCDD RLA DB
D SHIRES
M FRAUENHOFFER
J VINES